LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104380.D
Acq On : 9 Apr 2018 18:49
Operator : JU/SJ
Sample : J2157-05 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-040618-C

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.998	491	495	500	rVB	53228	56145	2.06%	0.267%
2	5.404	559	564	567	rBV	1314284	1153308	42.35%	5.492%
3	6.034	667	671	676	rBV	66555	70130	2.57%	0.334%
4	6.422	733	737	745	rBV	1217669	1178803	43.28%	5.614%
5	6.569	758	762	765	rBV	1447533	1201936	44.13%	5.724%
6	6.804	798	802	806	rVB	1229010	968664	35.57%	4.613%
7	6.957	825	828	832	rBV	1112664	951564	34.94%	4.531%
8	7.363	893	897	900	rBV	860021	687294	25.24%	3.273%
9	8.086	1015	1020	1024	rBV	1500936	1251054	45.94%	5.958%
10	9.045	1180	1183	1187	rVB3	30548	28183	1.03%	0.134%
11	9.163	1199	1203	1206	rBV	1785407	1327058	48.73%	6.320%
12	9.245	1213	1217	1221	rBV3	41114	47053	1.73%	0.224%
13	9.557	1266	1270	1273	rBV	149998	129490	4.75%	0.617%
14	9.775	1304	1307	1311	rVB	70297	56517	2.08%	0.269%
15	9.845	1315	1319	1322	rVV	1334627	1129038	41.46%	5.377%
16	10.275	1389	1392	1394	rVB	86241	65801	2.42%	0.313%
17	10.492	1424	1429	1435	rBV	31813	53308	1.96%	0.254%
18	10.627	1447	1452	1456	rBV	729503	596530	21.90%	2.841%
19	10.745	1469	1472	1480	rVB	87322	105841	3.89%	0.504%
20	11.198	1546	1549	1551	rBV	54379	45309	1.66%	0.216%
21	11.227	1551	1554	1560	rVB2	41004	45748	1.68%	0.218%
22	11.333	1568	1572	1574	rBV	1003766	933036	34.26%	4.443%
23	11.351	1574	1575	1578	rVV	139621	97175	3.57%	0.463%
24	11.404	1582	1584	1587	rVB	41666	31142	1.14%	0.148%
25	11.622	1618	1621	1624	rBV	42604	39036	1.43%	0.186%
26	11.727	1635	1639	1642	rBV	830214	676875	24.85%	3.223%
27	11.857	1658	1661	1665	rVB2	48005	44727	1.64%	0.213%
28	11.945	1673	1676	1678	rBV	33050	32290	1.19%	0.154%
29	12.033	1688	1691	1694	rBV	38593	38085	1.40%	0.181%
30	12.257	1726	1729	1735	rBV7	18995	32311	1.19%	0.154%
31	12.380	1747	1750	1752	rBV2	35008	30787	1.13%	0.147%
32	12.416	1752	1756	1758	rVV	2864946	2723500	100.00%	12.970%
33	12.439	1758	1760	1768	rVB2	1725928	1544735	56.72%	7.356%
34	12.521	1770	1774	1776	rVV	338533	291556	10.71%	1.388%

LSC Area Percent Report

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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-040618-C

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.545	1776	1778	1781	rVB	198907	156092	5.73%	0.743%
36	12.774	1811	1817	1819	rBV	189889	204488	7.51%	0.974%
37	12.916	1838	1841	1845	rBV	1059051	963659	35.38%	4.589%
38	13.104	1870	1873	1875	rVB	40447	33633	1.23%	0.160%
39	13.151	1879	1881	1882	rBV	37985	28136	1.03%	0.134%
40	13.168	1882	1884	1887	rVB	48812	38151	1.40%	0.182%
41	13.245	1895	1897	1901	rBV2	39721	33797	1.24%	0.161%
42	13.816	1992	1994	1998	rBV3	65646	78212	2.87%	0.372%
43	13.974	2017	2021	2024	rBV	1130537	1068075	39.22%	5.086%
44	15.439	2266	2270	2274	rBV	585688	730730	26.83%	3.480%

Sum of corrected areas: 20999002

LSC Report - Integrated Chromatogram

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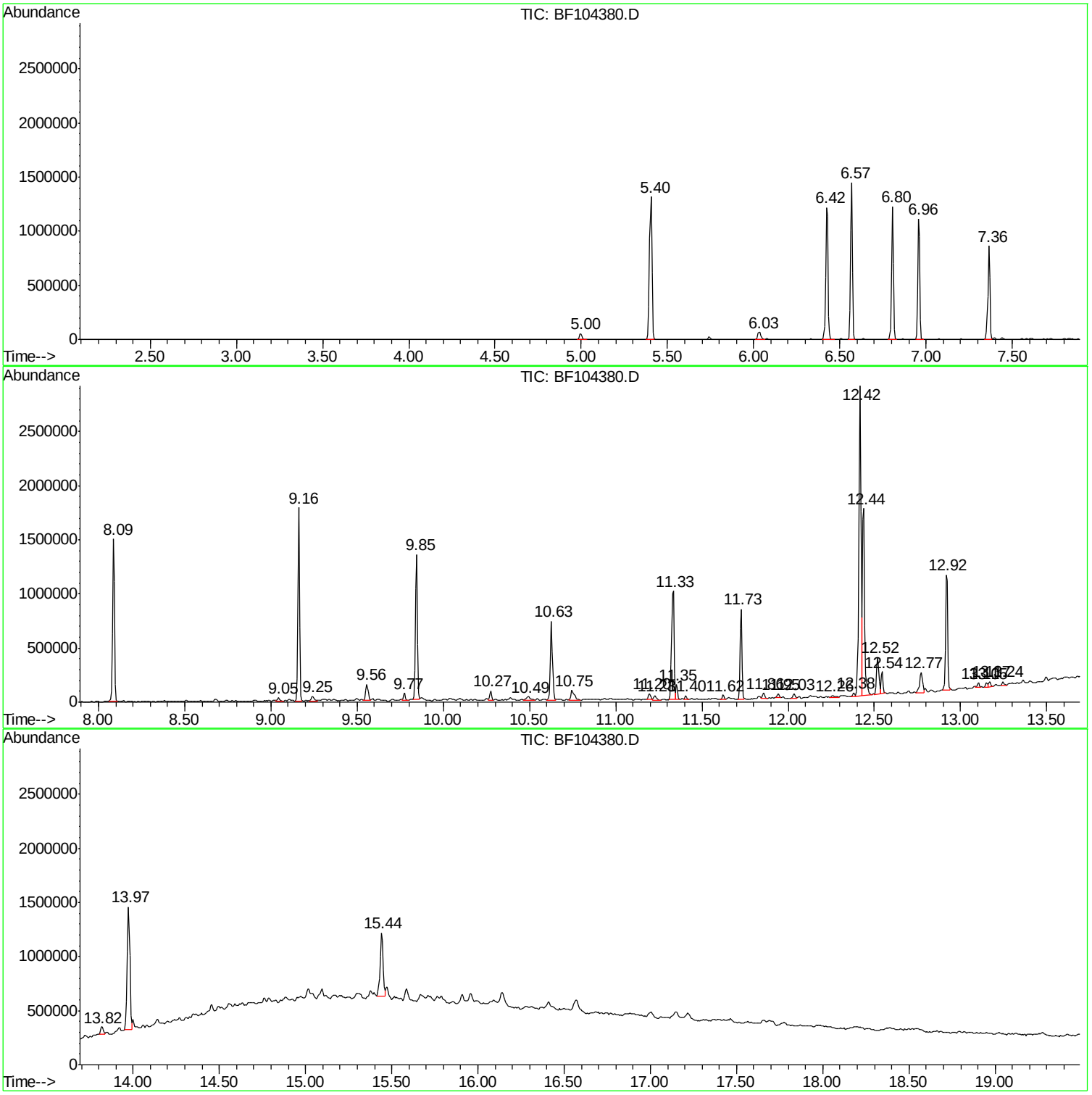
Acq On : 9 Apr 2018 18:49
Operator : JU/SJ
Sample : J2157-05 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104380.D
Acq On : 9 Apr 2018 18:49
Operator : JU/SJ
Sample : J2157-05 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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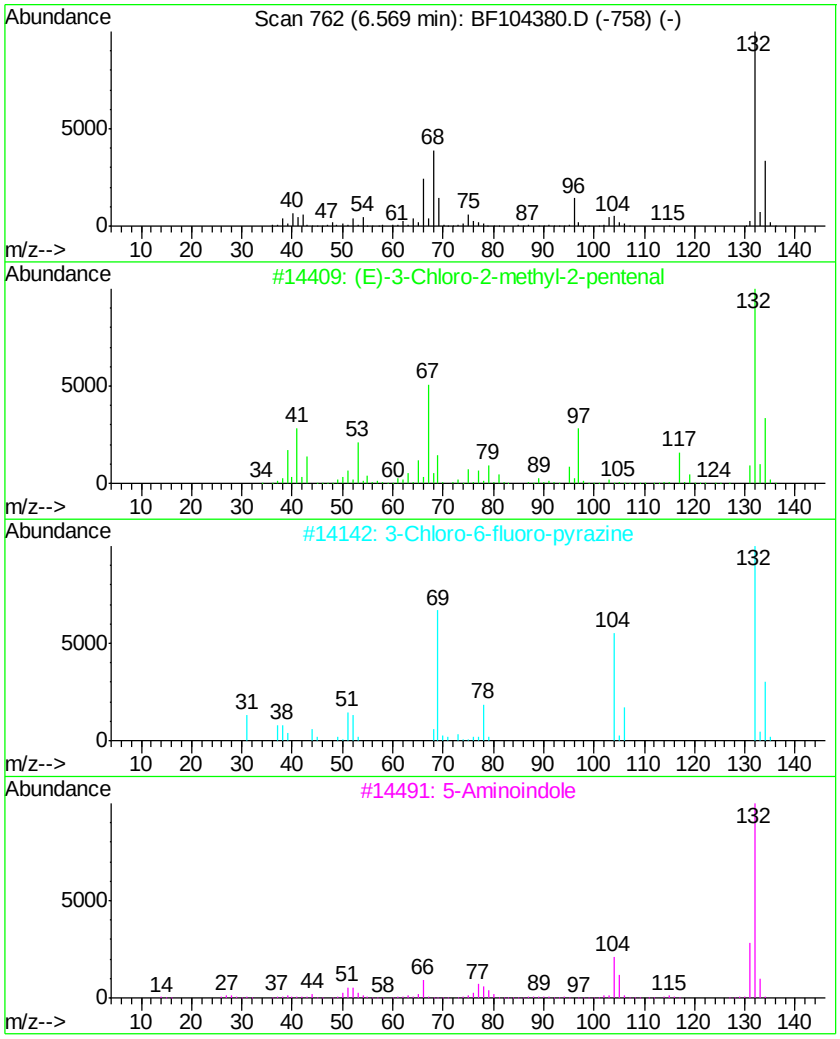
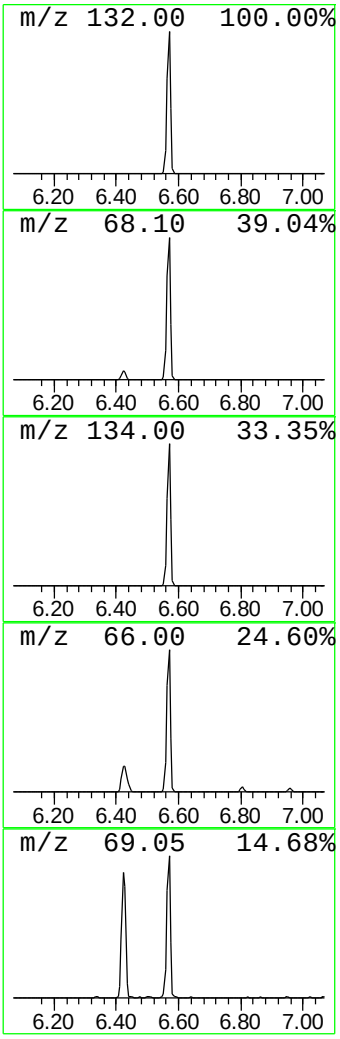
Peak Number 1 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	24.82 ng	1201940	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
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Acq On : 9 Apr 2018 18:49
Operator : JU/SJ
Sample : J2157-05 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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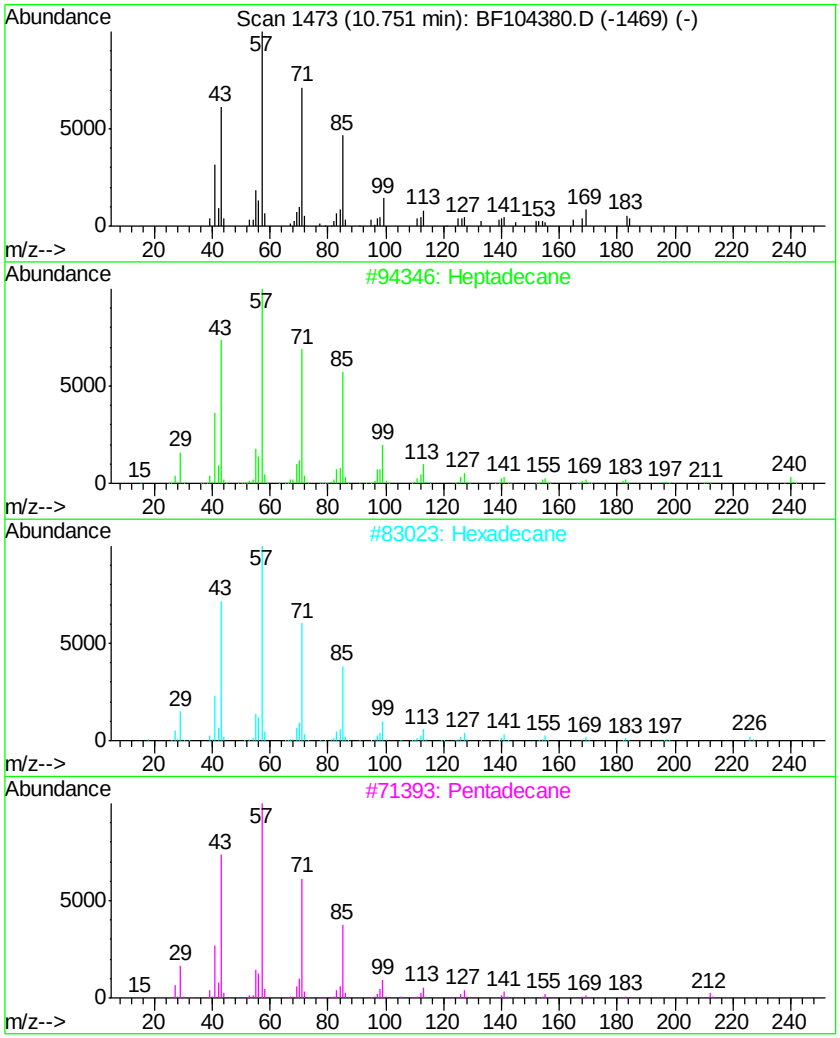
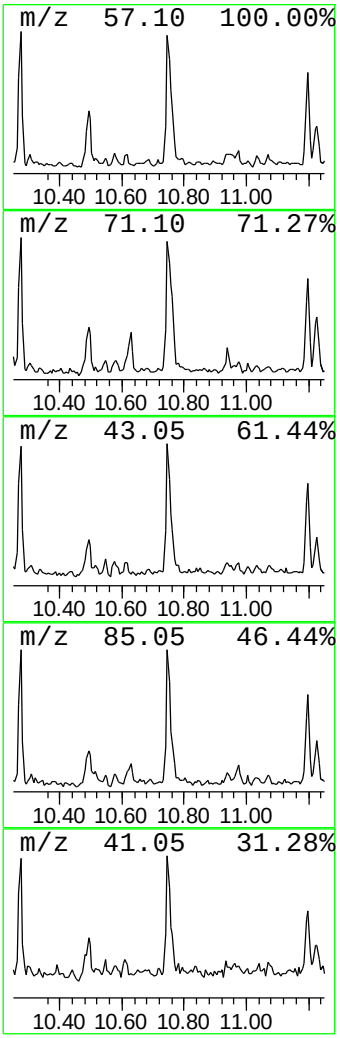
Peak Number 3 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.27 ng	105841	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Pentadecane	212	C15H32	000629-62-9	87
4	Octacosane	394	C28H58	000630-02-4	86
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
Data File : BF104380.D
Acq On : 9 Apr 2018 18:49
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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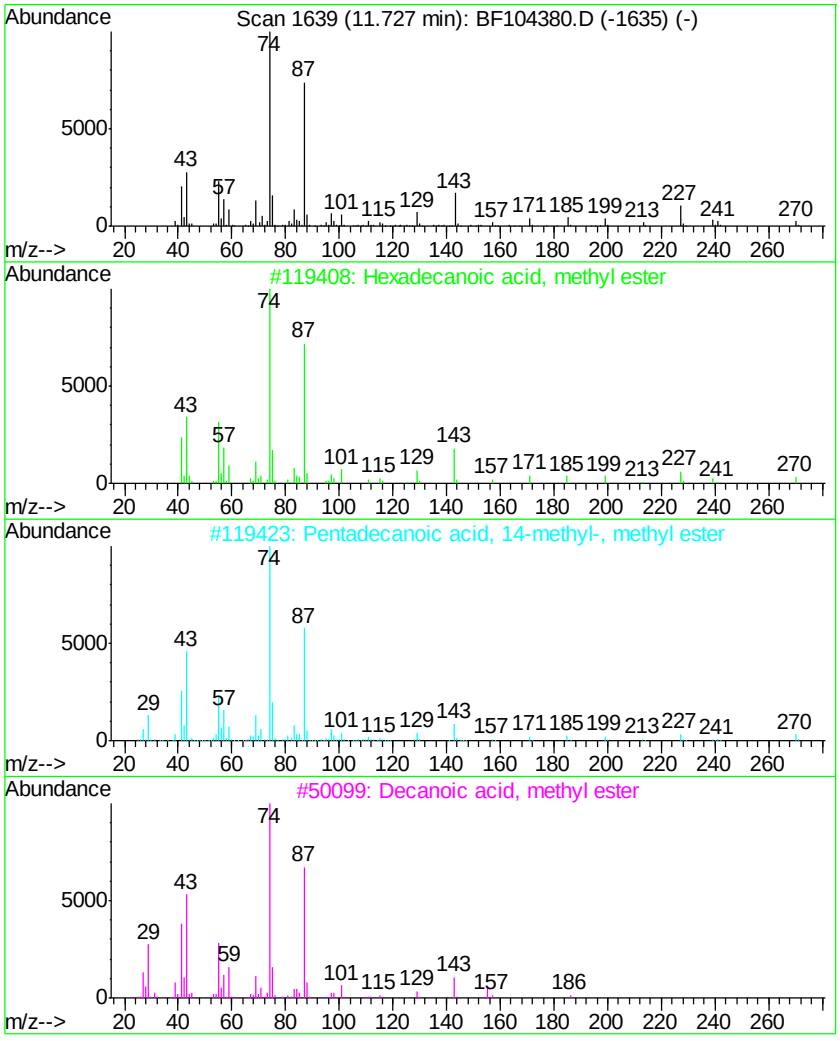
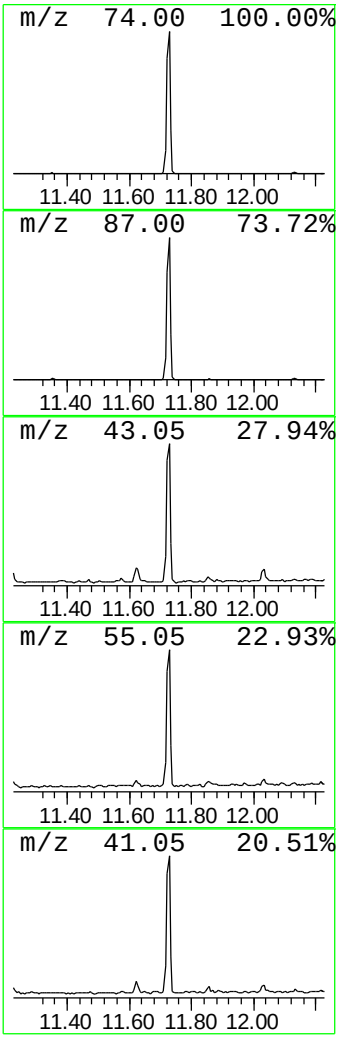
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	14.51 ng	676875	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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Acq On : 9 Apr 2018 18:49
Operator : JU/SJ
Sample : J2157-05 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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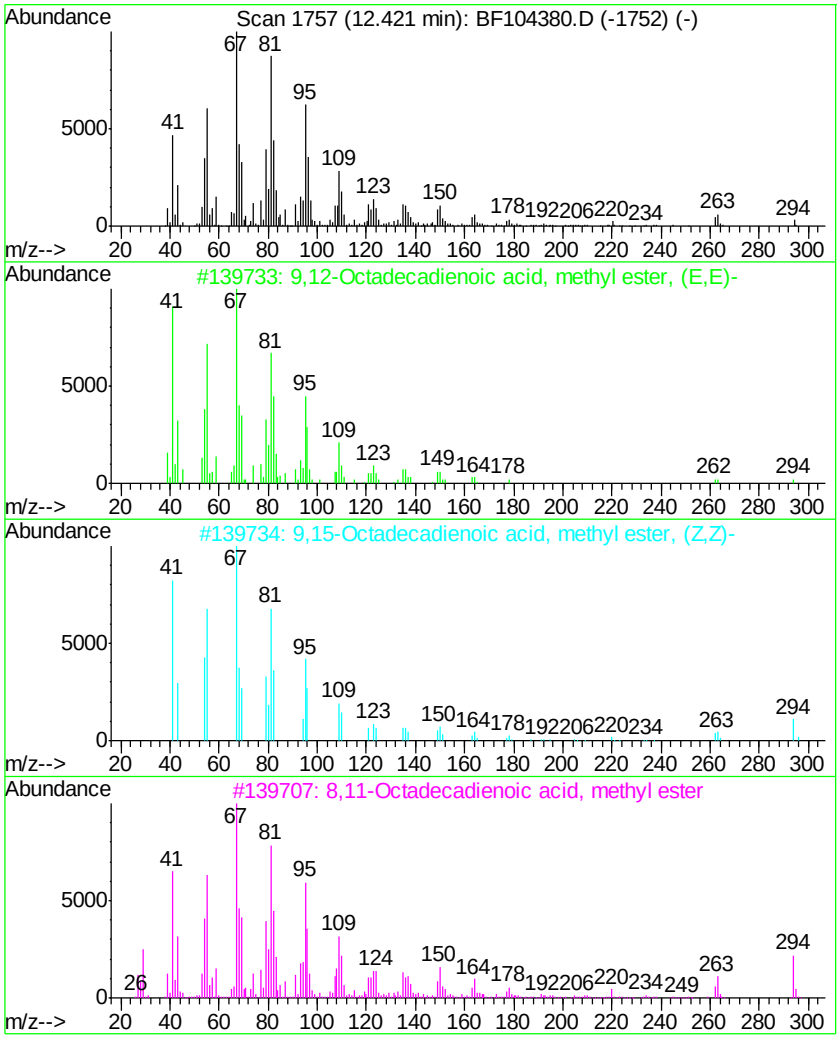
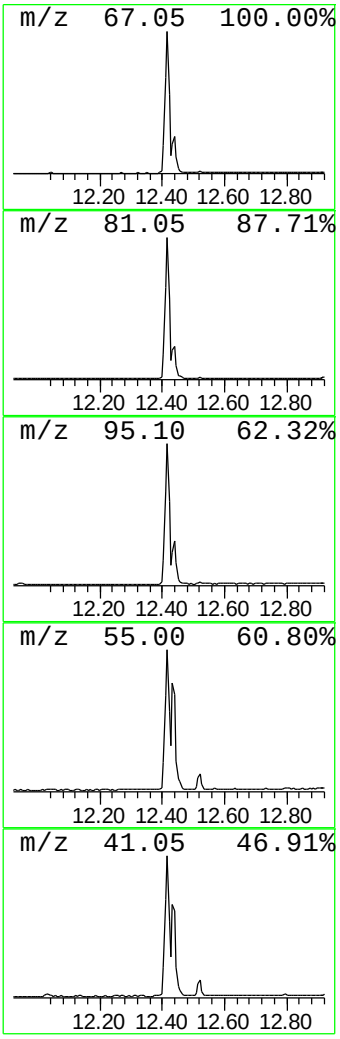
Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	58.38 ng	2723500	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	98





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040918\
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Acq On : 9 Apr 2018 18:49
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-040618-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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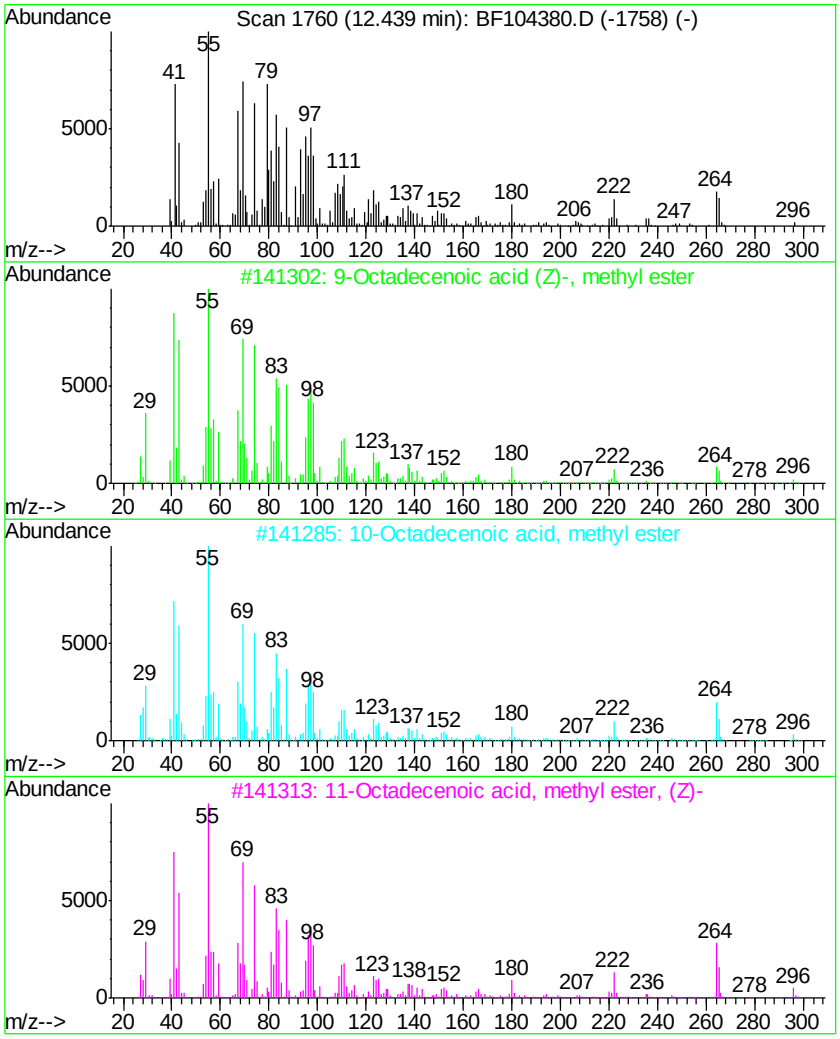
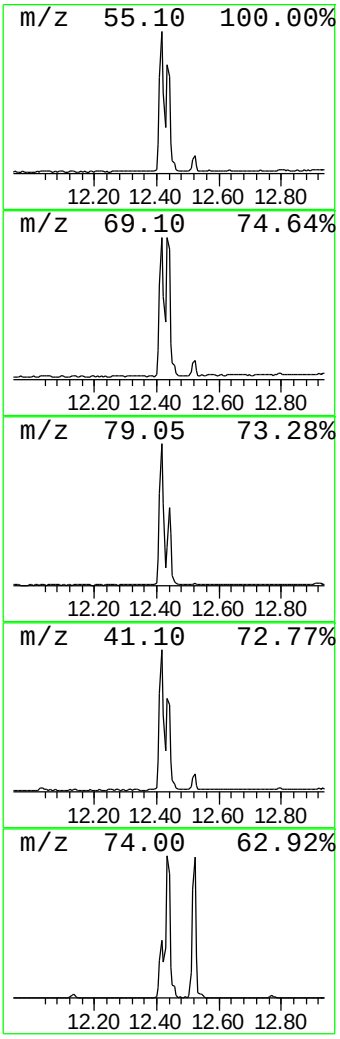
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	33.11 ng	1544740	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	97
3	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	97
4	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	97
5	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	97





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.57	6.57	24.8	ng	1201940	1	6.80	968664	20.0
Heptadecane	10.75	2.3	ng	105841	4	11.33	933036	20.0
Hexadecanoic acid...	11.73	14.5	ng	676875	4	11.33	933036	20.0
9,12-Octadecadien...	12.42	58.4	ng	2723500	4	11.33	933036	20.0
9-Octadecenoic ac...	12.44	33.1	ng	1544740	4	11.33	933036	20.0